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A UNIFIED THEORY OF SOLID PROPELLANT IGNITION. PART 2. COMPUTER PROGRAM

H. H. Bradley, Jr.

Naval Weapons Center
China Lake, California

August 1974

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FOREWORD

This report was prepared as part of a research program at the Naval Weapons Center on the subject of Ignition of Solid Propellant Rockets, sponsored under Naval Ordnance System Command Task Assignment ORD-331-001/200-1/UR024-02-02. Previous reports include an extensive summary of the then current status of various theories of solid propellant ignition (NAVWEPS Report 8987, NOTS TP 3954), and extended analyses of solid phase theory (NWC TP 4618) and heterogeneous theory (NWC TP 4864). The present report is the second of a series of three reports on a Unified Theory of Solid Propellant Ignition. It deals with the computer program developed to solve the mathematical model developed in the first report of the series (NWC TP 5618, Part 1). Part 3 on the results of a parameter study is published separately.

This report has been prepared for timely presentation of information. Because of the continuing nature of research in this area, refinements may be made in the future.

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(U) A Unified Theory of Solid Propellant Ignition. Part 2. Computer Program , by H. H. Bradley, Jr., Naval Weapons Center, China Lake, Calif., August 1974, 30 pp. (NWC TP 5618, Part 2, publication UNCLASSIFIED.)

(U) A computer code is presented for solving the equations of the unified solid propellant ignition theory reported in Part 1 of this series of reports. The computing algorithm is based upon a predictor-corrector version of the Crank-Nicholson implicit method applied to the system of parabolic partial differential equations. Coding is in FORTRAN V language. Use is made of PARAMETER statements to effect variable dimensions and of NAMELIST statements for convenience in data input. Internal subroutines are freely utilized to overcome increased computer times which attend the use of argument lists associated with external subprograms. Approximately twenty-three thousand decimal locations are required for the compiled program, not including plotting routines, which would be dependent upon a particular computer installation.

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NOMENCLATURE

(See Table 1 for definitions relevant to data input quantities)

A_i $\begin{cases} \alpha_g/\rho_{go} & : i = 1\text{-}9, 13 \text{ (gas)} \\ \alpha_c/\rho_{co} & : i = 10\text{-}12, 14 \text{ (solid)} \end{cases}$

B_i $\begin{cases} LcA_i\rho_g\lambda_g/C_g & : i = 1\text{-}9 \\ 0 & : i = 10\text{-}12 \\ B_i/Le & : i = 13 \\ \alpha_c\lambda_c/C_c & : i = 14 \end{cases}$

a_{ij}, b_{ij}, c_{ij}, d_{ij} *Defined in Eq. B4-B7*

$f_{1i}(\phi_j)$ $\begin{cases} A_iB_i\ (1 + \phi_j)^2 & : \text{solid} \\ A_iB_i\ (1 - \phi_j)^2 & : \text{gas} \end{cases}$

$f_{2i}(\phi_j)$ $\begin{cases} A_i\ (1 + \phi_j) & : \text{solid} \\ A_i\ (1 - \phi_j) & : \text{gas} \end{cases}$

$g_i(u_s)$ $\begin{cases} m_s - B_i & : \text{solid} \\ m_s + B_i & : \text{gas} \end{cases}$

$h_i(\phi_j)$ *Volumetric source of quantity i at node j*

1. INTRODUCTION

The governing equations of a unifird theory of solid propellant ignition were developed (see Footnote 1) and are summarized in Appendix A. Because of the occurrence of the nonlinear source terms V and S and of the surface regression m_S there is little chance for the existence of an exact analytic solution of the general set of equations. Simple sub-theories have been successfully handled by approximate methods such as matched asymptotic expansions[2] and local similarity[3]; it is not unlikely that other, as yet untreated, sub-theories may eventually yield to comparable techniques.

There are two general approaches to the acquisition of solutions to the unsolved sub-theories: (1) development of special methods, either numerical or approximate analytic, for handling each sub-theory in an optimum manner and (2) development of a generalized numerical program. The latter course is followed here. Even though this approach leads to a much more complicated computer program, it has the advantage of greater flexibility.

2. CHOICE OF METHOD OF SOLUTION

In addition to the approximate analytic techniques already mentioned, there are a great number of numerical methods for obtaining solutions to partial differential equations. These methods fall generally into two classes: (1) direct replacement of the derivatives by appropriate finite difference analogs and (2) use of an indirect approach, typified by the methods of weighted residuals,[4-5] which often leads to a finite difference

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[1] Naval Weapons Center. *A Unified Theory of Solid Propellant Ignition; Part 1 - Development of Mathematical Model,* H. H. Bradley, Jr., China Lake, CA, NWC August 1974 (NWC TP 5618, Part 1).

[2] Linan, A., and F. A. Williams. "Radiant Ignition of a Reactive Solid with In-Depth Absorption," COMBUS AND FLAME, Vol. 18 (1972), pp. 85-97.

[3] Waldman, Cye H. "Theory of the Heterogeneous Ignition," COMB SCI TECH, Vol. 2 (1970), pp. 81-93.

[4] Finlayson, B. A., and L. E. Scriven. "The Method of Weighted Residuals --A Review," APPL MECH REV, Vol. 19, No. 1 (September 1966), pp. 735-48.

[5] Crandall, S. H. *Engineering Analysis, A Survey of Numerical Procedures.* New York, McGraw-Hill Book Co., 1956.

formulation. The latter results in a smoothing effect which may tend to obscure details of solutions varying rapidly with position unless many weighting functions are used. In addition, the algebraic manipulations become somewhat tedious for large systems. In applying the direct finite difference methods, care is essential to avoid numerical instabilities which often obscure the true solution.

Three possibilities exist in the direct application of finite difference techniques to the set of parabolic equations of the unified ignition theory depending upon whether one or both independent variables (time and space) are subjected to finite difference operations.[6] Differencing in the time direction (often referred to as the method of lines) produces a large system of simultaneous ordinary differential equations which are stiff by nature. Some special methods, such as Gear's,[7] are available for solution of such systems; good stability and accuracy with reasonable computing times are bought at the expense of very large computer requirements. The final method, differencing along both the time and space axes, can be carried out either explicitly or implicitly. In most explicit methods, computing parameters are severely limited owing to stability considerations, resulting in excessive computing times. In general, implicit methods are more stable but require the solution of simultaneous nonlinear algebraic equations; nevertheless, the special form of the system matrix after linearization through iterative or predictor-corrector methods makes the implicit approach more attractive. Two versions of the implicit method will be described, differing principally in the treatment of the nonlinear terms. The computer code is implemented for one method and may easily be extended to the other version.

3. DESCRIPTION OF COMPUTING ALGORITHMS

3.1 FIELD EQUATIONS

The equations to be solved are displayed in Appendix A. For convenience in describing the computing algorithm, the field equations (Eq. A1 - A2) may be written compactly as:

$$\frac{\partial v}{\partial t} = f_1(\phi)\,\frac{\partial^2 v}{\partial \phi^2} + f_2(\phi)\,g\left(v_s\right)\,\frac{\partial v}{\partial \phi} + h(v) \qquad (1)$$

---

[6] Crank, J., and P. Nicholson. "A Practical Method for Numerical Evaluation of Solutions of Partial Differential Equations of the Heat-Conduction Type," CAMBRIDGE PHIL SOC, PROC, MATH PHYS SCI, Vol. 43 (1947), pp. 50-67.

[7] Gear, C. W. *Numerical Initial Value Problems in Ordinary Differential Equations.* Englewood Cliffs, N. J. Prentice-Hall, 1971. 253 pp.

In Eq. (1), v represents the vector dependent variable with mass fraction and enthalpy as scalar components; f_1 and f_2 are functions of position (nodal index) only which arise from the coordinate transformation;[1] $g(v_s)$ is a nonlinear function of v evaluated at the phase interface, and h is a nonlinear function of v (hence of ϕ) evaluated in the bulk phase. Using central differences to approximate the first and second derivatives we obtain:

$$\left(u_j^{k+1} - u_j^o\right)/\Delta t = f_1\left(\phi_j\right)\Delta_\phi^2\left[\theta u_j^{k+1} + (1-\theta)u_j^o\right]$$

$$+ f_2\left(\phi_j\right)\delta_\phi\left[\theta u_j^{k+1} + (1-\theta)u_j^o\right]\bar{g}\left(u_s\right) + \bar{h}\left(u_j\right) \qquad (2)$$

where the difference operators are defined as:

$$\Delta_\phi^2 w_j \equiv \left(w_{j+1} - 2w_j + w_{j-1}\right)/(\Delta\phi)^2 \qquad (3)$$

$$\delta_\phi w_j \equiv \left(w_{j+1} - w_{j-1}\right)/2\Delta\phi \qquad (4)$$

Equation (2) represents a general three point algorithm for advancing the solution from time t through the interval Δt. The superscripts o and $k+1$ denote approximations to the true solution v at the space node j corresponding to the times t and $t+\Delta t$, respectively. The terms $\bar{g}$ and $\bar{h}$ represent appropriately chosen values of g and h for the interval Δt. The parameter θ determines whether the algorithm is fully implicit (backward difference algorithm, $\theta=1$) or explicit ($\theta=0$). Intermediate values of θ may be chosen, $\theta=1/2$, corresponding to the Crank-Nicholson scheme, being the most common. The explicit scheme, with g and h evaluated at the current time, t, leads to linear algebraic equations which may be solved immediately for the u^{k+1}; however, stability considerations severely restrict its use. All other schemes (stability is possible only when $\theta \geq 1/2$) generate systems of simultaneous, algebraic equations involving values of u^{k+1} at three nodes per equation (except at the boundaries, to be discussed later). The nonlinearities of the system in the present application may be handled by any of a number of linearization techniques, examples of which are described in the following sections.

3.1.1 Iterative

The parameter θ, which determines the degree to which the finite difference approximation is implicit or explicit, is also a weighting function for the derivatives evaluated at the current and advanced times. It seems

logical to apply a weighting function to the nonlinear functions g and h. If the same weighting function is used, then

$$\bar{g}\left(u_s\right) = g\left[\theta u_s^k + (1-\theta)u_s^o\right] \tag{5}$$

$$\bar{h}\left(u_j\right) = h\left[\theta u_j^k + (1-\theta)u_j^o\right] \tag{6}$$

where the superscript k denotes the previous approximation to the unknown function at $t + \Delta t$. It may be obtained by extrapolation from earlier values of the solution or by simply using the value of the function at t as a first approximation. The resulting iterative process (Picard's) is linearly convergent. A more sophisticated, quadratically convergent iteration (Newton's) involves a series expansion of the functions u_s^k and u_j^k with the linear terms being retained.[8] In the current application, it is believed that the number of evaluations of complicated functions required by this latter method would increase computing times more than is warranted.

3.1.2 Predictor-Corrector

The algorithm actually utilized in the computer coding consists essentially of a Crank-Nicolson step of Δt with nonlinear functions of dependent variables evaluated at $\Delta t/2$. These latter values are first estimated by an implicit predictor step ($\theta=1$) of $\Delta t/2$.[9] We thus have for the predictor:

$$k = 0,\ \theta = 1,\ \Delta t \rightarrow \Delta t/2$$

and for the Crank-Nicholson corrector

$$k = 1,\ \theta = 1/2,\ \Delta t \rightarrow \Delta t$$

where

$$\bar{g}(u_s) = g(u_s^k)$$

$$\bar{h}(u_j) = h(u_j^k)$$

---

[8] Ames, William F. *Numerical Methods for Partial Differential Equations.* London, Thomas Nelson and Sons, Ltd., 1969.

[9] Douglas, J., and B. F. Jones. "On Predictor-Corrector Methods for Non-Linear Parabolic Differential Equations, SOC IND APPL MATH, J. Vol. 11, No. 1 (March 1963), pp. 195-204.

When the above relationships are substituted into Eq. (2), the predictor becomes

$$\frac{u_j^1 - u_j^o}{\Delta t/2} = f_{1i}\left(\phi_j\right)\Delta_\phi^2\left(u_j^1\right) + f_{2i}\left(\phi_j\right)\delta_\phi\left(u_j^1\right)g_i\left(u_s^o\right) + h\left(u_j^o\right) \qquad (7)$$

and the corrector,

$$\frac{u_j^2 - u_j^o}{\Delta t} = f_{1i}\left(\phi_j\right)\Delta_\phi^2\left(u_j^2 + u_j^o\right)/2 + f_{2i}\left(\phi_j\right)\delta_\phi\left(u_j^2 + u_j^o\right)g_i\left(u_s^1\right)/2 + h\left(u_j^1\right) \qquad (8)$$

3.2 INTERFACE EQUATIONS

The matching conditions at the phase interface (Eq. A3 and A4) contain derivatives of the unknowns (except solid species concentration) at the interface as well as values of the unknowns. Using central differences at the boundary ($j=1$) introduces fictitious gaseous and solid nodal points. If it is assumed that the field equations also are valid at the boundary, the same fictitious nodal values are introduced into the difference analog of the field equations. The fictitious values may, therefore be eliminated, leading to a system of simultaneous equations in tridiagonal form to be solved for the values of the unknowns at the nodal points. Details are shown in Appendix B.

Special treatment is required for the solid species because the space derivative of concentration of solid species does not appear in a boundary condition. Hence, there is no second equation by which fictitious nodal values may be eliminated as in the case of enthalpy and gas phase concentrations. To resolve the problem, a one-sided, three-point finite difference analog is used for the first space derivative of solid phase species.

In the application of the predictor-corrector algorithm to the boundary equations, a backward difference equation replaces the Crank-Nicholson form for both steps of the algorithm to avoid instabilities which can be incurred by using the Crank-Nicholson method with derivative boundary conditions.[10] It is not known whether the instability would arise in the predictor-corrector technique as well; however, the precaution was taken until further investigations could be completed.

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[10] Douglas, J. "A Survey of Numerical Methods for Parabolic Differential Equations," in *ADVANCE COMPUTER*, New York, Academic Press, 1961. Vol II, pp. 1-54.

4. DESCRIPTION OF COMPUTER PROGRAM

The computer program was designed to take advantage of the capabilities of the Univac 1108 Exec 8 system at the Naval Weapons Center. Coding is in FORTRAN V language, use being made of PARAMETER and NAMELIST statements and internal subprograms.

The input to the computer program consists of the assignments for 116 quantities representing physical parameters, program controls, and output specifications. To simplify program use, standard, or base values are assigned to 80 of these quantities (see Table 1); other than base values are introduced by way of a NAMELIST statement. The remaining 36 quantities are specified through conventional input methods.

The solution of the equations includes values of the fourteen dependent variables at each time interval and each space node of the computing mesh. Since a minimum of 100 nodes has been selected to assure accuracy, the total output of a run of 100 to 300 time steps would represent an overwhelming volume of printout. As a compromise, only a fraction of the computed output is printed during the initial program execution; selection of the printed portion is controlled by input parameters. To avoid loss of the unprinted solution, the entire solution is stored on tape, through intermediate use of high speed mass storage, for later processing and analysis, which may include plotting or additional printing of results.

4.1 FLOW CHART

A simplified flow chart of the program is shown in Figure 1. A complete listing of the program is available. Address Commander, Naval Weapons Center, Code 608, China Lake, CA 93555. The contents of each block is briefly provided in the following descriptions.

PROGRAM INITIALIZATION - Contains specification statements such as array dimensions, formats, data statements (including specification of the values of the base set of 80 parameters), and several program constants. The output mass storage file is defined into which the complete solution is to be stored (ISF=10). This unit number may be changed to conform to local computer requirements. In the current coding, only one such file may be generated per program execution.

RUN INITIALIZATION - (1) Saves the standard parameter set for later restoration. This provision is included to allow several runs to be stacked and would require definition of an equivalent number of storage files. (2) Uses NAMELIST input to alter selected base parameters; uses standard input (READ) statements for specifying run identification and output print controls.

TABLE 1. NAMELIST Input Parameters and Standard Values.

Computer designation	Algebraic designation	Standard value	Definition
FREQ 1	ν_1	0.	Pre-exponential factor, reaction 10[a]
FREQ 5	ν_5	0.	Pre-exponential factor, reaction 5[b]
FREQ 6	ν_6	0.	Pre-exponential factor, reaction 6[c]
FREQ 7	ν_7	0.	Pre-exponential factor, reaction 7[d]
FREQ 8	ν_8	0.	Pre-exponential factor, reaction 8[e]
FREQ 10	ν_{10}	0.	Pre-exponential factor, solid fuel vaporization
FREQ 11	ν_{11}	0.	Pre-exponential factor, solid oxidizer vaporization
FREQ 12	ν_{12}	0.	Pre-exponential factor, solid product vaporization
E1	E_1	0.	
E5	E_5	0.	
E6	E_6	0.	Activation energy. Subscripts correspond to those for pre-exponential factors.
E7	E_7	0.	
E8	E_8	0.	
E10	E_{10}	0.	
E11	E_{11}	0.	
E12	E_{12}	0.	
Q1	Q_1	0.	
Q5	Q_5	0.	
Q6	Q_6	0.	
Q7	Q_7	0.	Heat of reaction (positive for exothermic). Subscripts correspond to those for pre-exponential factors.
Q8	Q_8	0.	
Q10	Q_{10}	0.	
Q11	Q_{11}	0.	
Q12	Q_{12}	0.	

TABLE 1. (Contd.)

Computer designation	Algebraic designation	Standard value	Definition
VF7	VF_7	1.	Fuel reaction order, reaction 7
VO7	VO_7	1.	Oxidizer reaction order, reaction 7
VF8	VF_8	1.	Fuel reaction order, reaction 8
VO8	VO_8	1.	Oxidizer reaction order, reaction 8
SO5	S_5	1.	Oxidizer reaction order, reaction 5
SO6	S_6	1.	Oxidizer reaction order, reaction 6
STOV2	b_2	1.	Oxidizer stoichiometry, reaction 7
STOV4	b_4	1.	Oxidizer stoichiometry, reaction 8
STOV 11	b_{11}	1.	Oxidizer stoichiometry, reaction 10
STOS2	b_2'	1.	Oxidizer stoichiometry, reaction 5
STOS4	b_4'	1.	Oxidizer stoichiometry, reaction 6
MU1	μ_1	1.	Mol. wt. of vaporized solid fuel[f]
MU2	μ_2	1.	Mol. wt. of vaporized solid oxidizer
MU4	μ_4	1.	Mol. wt. of original gaseous oxidizer
MU5	μ_5	1.	Mol. wt. of product in reaction 5
MU6	μ_6	1.	Mol. wt. of product in reaction 6
MU7	μ_7	1.	Mol. wt. of product in reaction 7
MU8	μ_8	1.	Mol. wt. of product in reaction 8
MU9	μ_9	1.	Mol. wt. of inert gaseous diluent
MU10	μ_{10}	1.	Mol. wt. of solid fuel
MU11	μ_{11}	1.	Mol. wt. of solid oxidizer
MU12	μ_{12}	1.	Mol. wt. of solid product
COND (1)	λ_c	1.	Solid thermal conductivity (cal/cm sec deg K)
COND (2)	λ_g	1.	Gas thermal conductivity
SPHT (1)	C_c	1.	Solid specific heat (cal/gm deg K)
SPHT (2)	C_g	1.	Gas specific heat (cal/gm deg K)

TABLE 1. (Contd.)

Computer designation	Algebraic designation	Standard value	Definition
RHO1	ρ_{co}	1.	Solid density (gm/cm^3)
LE	Le	1.	Lewis number of gas = $\rho CD/\lambda$
BE	β	1.	Solid extinction coefficient cm^{-1}
TLIM(1)	T_{co}	1.	Initial solid temperature ^oK
TLIM(2)	T_{go}	1.	Initial gas temperature ^oK
PRESS	p	82.05	Pressure (atmospheres)
YFZ1	Y_{fc}	1.	Initial gas fuel mass fraction[g]
YOZ2	Y_{og}	1.	Initial gas oxidizer mass fraction
QDOT	q_r	1.	Radiant flux (cal/cm^2 sec)
TMELIM		10.	Ignition time limit (sec)
TSLIM		3.	Ignition temperature limit (deg K)
FCT		2.	One greater than number of heating periods allowed for ignition after cutoff
NREFIR		0.	Number of refires allowed to achieve ignition in cutoff case
TCO		11.	Time to first cutoff
CUTOFF		F	Cutoff flag: F = no cutoff T = cutoff
SUB		F	Subsurface absorption flag: F = no SSA T = SSA
REG		F	Surface regression flag: F = no regression T = regression
ALP(1)	α_c	1.	X-scale transformation for solid
ALP(2)	α_g	1.	X-scale transformation for gas
N(1)	N_c	NNN-1	Number of strips in solid
N(2)	N_g	NNN-1	Number of strips in gas

TABLE 1. (Contd.)

Computer designation	Algebraic designation	Standard value	Definition
DULIM		.01	DULIM $\geq$ T/T in search for time step
DLLIM		.005	DLLIM $\leq$ T/T in search for time step
SPRO5		0	Flag for including reaction 5*
SPRO6		0	Flag for including reaction 6*
SPRO10		0	Flag for including solid fuel pyrolysis*
SPRO11		0	Flag for including solid oxidizer pyrolysis*
SPRO12		0	Flag for including solid product pyrolysis*
NHLIM		10	Number of time step halvings allowed in search for time step
SURF		F	Flag for all surface processes F - ignore, T - include

a Solid Reaction: $[F] + b_{11}'[o] = b_{12}[P]$

b Surface Reaction: $[F] + b_2'[o] = b_5[P]$

c Surface Reaction $[F] + b_4'[o] = b_6[P]$

d Gas Reaction: $[F] + b_2[o] = b_7[P]$

e Gas Reaction: $[F] + b_4[o] = b_8[P]$

f Set all molecular weights equal in this version of the computer program

g Set Y_{fc} to any negative value to obtain reverse of reaction 10. Then the program will set $Y_{pc} = 1.$ and $Y_{fc} = Y_{oc} = 0.$ Also ν_1 must be set negative, and Q_1 becomes negative for exothermic reaction.

*Equals 0, do not include process; equals 1, include process.

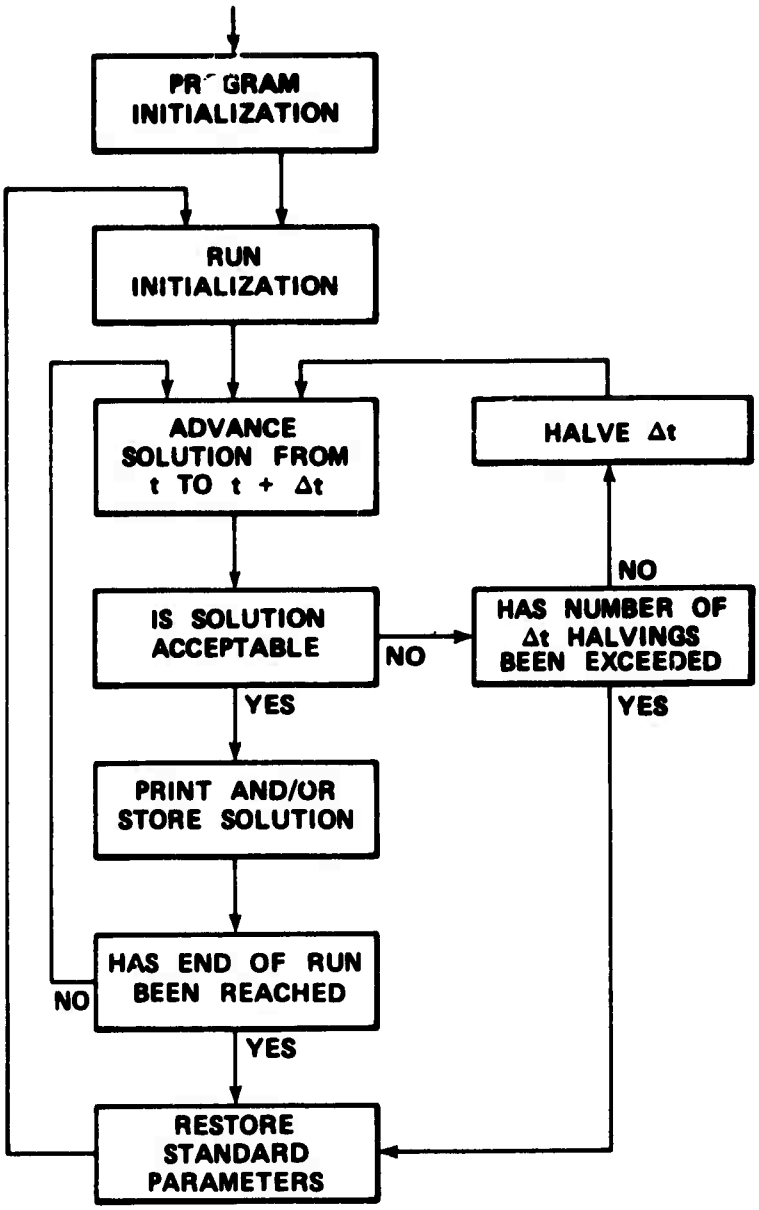

FIGURE 1. Simplified Flow Chart of Computer Program.

(3) Prints and (optionally) stores the run identification and parameters. (4) Calls subroutine START to compute run constants from input parameters and to estimate initial time step for integration. (5) Calls subroutine TSUB to convert enthalpies to temperatures. Prints and (optionally) stores initial conditions. (6) Calls subroutine ANFORM to evaluate solution at end of first time step by analytical formula from which nonlinear terms and effects of subsurface absorption are omitted. The subroutine ERCS is called to evaluate the error functions occurring in the analytic solution. It also prints and (optionally) stores the analytic step.

ADVANCE SOLUTION FROM t TO t + Δt - This segment of coding contains (through subroutines ABCCOE, DCOE, TRIDAG, SPEC, S, VOL, AND S1314) the implicit/Crank-Nicholson predictor-corrector algorithm. Program flow is directed in accordance with input options.

TEST ACCEPTABILITY OF SOLUTION - Subroutine CRIT contains the coding which ascertains the acceptability of the solution after each time step. Criteria examined are: (1) non-negativity of concentration and (2) bracketing of the time rate of change of temperature between upper and lower absolute limits. If a criterion is violated the time step is halved or doubled as appropriate and the step repeated. This step size adjustment is not invoked until after the first ten steps and is then limited to a number of halvings as specified by an input control parameter. When this number is equalled the run is terminated. In addition, CRIT controls the go/no-go computations as follows:

(a) Constant heat flux is applied until a specified time, when the flux is reduced to zero. The solution at that time is saved.

(b) The solution is continued with zero flux for a specified time interval after shutoff.

(c) If the temperatures at the surface and at the first ten gas nodes are decreasing after the above specified time interval, then the saved cutoff values are restored, and heating is continued for one more time step before another shutoff is invoked. Steps (b) and (c) are then repeated. The search for ignition, as evidenced by an increase in temperature at the surface or at one or more of the first ten gas nodes, is continued for a specified number of trials before the entire run is terminated.

OUTPUT SOLUTION - Prints solution after a specified number of time steps and space nodes (not necessarily equal increments) and stores (optionally) the entire solution after every time step.

END OF RUN - When specified heating time or surface temperature is reached, the base parameter set is restored and a new run may be started.

4.2 PROGRAM INPUT

(a) First two cards (Columns 2-80). Any message, identification, or special notes concerning the run. The information contained is stored on the mass storage file when the appropriate option is used, and would be valuable in the process of file searching during data retrieval.

(b) As mentioned in earlier sections, the program in its current form requires the specification of 116 quantities for its execution. To facilitate the preparation of input, standard values are assigned (through a DATA statement) to 80 quantities, which are listed in Table 1. By the use of the NAMELIST Provision, any combination of values of the 80 quantities may be modified by simply specifying the new values. Details of using NAMELIST are available at computer sites which utilizes a FORTRAN V compiler. If NAMELIST is not available, the input statements must be modified by substituting conventional coding with formatted READ statements.

(c) Final card (format 14I1, 1X, 15I3, 6I1, F6.0) used with a conventional READ statement to input the following controls:

ICALC (Columns 1-14) - a fourteen-element, single-digit integer vector which determines which of the dependent variables are to be computed. When ICALC(I) is set equal to zero, calculations for dependent variable I are bypassed, otherwise the calculation is made. ICALC(14) is set to one by the program, therefore, solid phase temperatures are always calculated.

NC (Columns 16-36) - a seven-element, array specifying the solid phase nodes to be printed out. The nodes are counted from the surface as number one and increase leftward into the solid phase. No decimal point should be punched. Right justify the integers in the appropriate fields. No integer exceeding the total number of solid nodes should be punched (101 as currently programmed).

NG (Columns 37-57) - Similar to NC except for gas phase nodes. Counting is from the surface as the number one gas node (hence, duplicating the number one solid node) and proceeding rightward. The same precautions apply.

NPINT (Columns 58-60) - Frequency of printout (timewise). NPINT = 0 or 1 prints every step; NPINT = 10 every tenth step, etc.

NCDENS (Column 61) - Control specifying mode of computing gas phase density.

OUTST (Column 62) - Control integer to cause solution to be stored on unit ISF. (ISF = 10 in coding.) Must not be zero or blank if storage is desired.

OUTPL (Column 63) - Control integer to provide on line printer plotting. Invokes subroutine PLOTTT, details of which would be dependent on local facilities. Since PLOTTT is now vacuous, OUTPL has no effect and may be left blank.

NER (Columns 64-66) - Diagnostic debug print controls. Leave blank.

FMDT (Columns 67-72, Format F6.0) - Factor by which initial estimated time step is multiplied in attempt to achieve starting accuracy. Now used as 1.0. Will be set to 1.0 if left blank or assigned a value less than 0.001

4.3 PROGRAM OUTPUT

The first page of printed output contains the message input on the first two cards, followed by a matrix listing of the 80 NAMELIST quantities and the program controls. On the succeeding pages the solution is arranged five time steps to the page. A sample printout is shown in Appendix C and is self explanatory except for the abbreviations. The line identifying the time also gives the stimulating energy flux and average surface mass fluxes for the time interval with the starting value TIME; also provided is the number of times the integration interval was halved to satisfy the acceptance criterion of subroutine CRIT. The first line following the time records a reduced temperature $(T-T_O)/T_O$ for specified nodes of the solid and gas phases. Succeeding lines contain species mass fractions. In general, solid nodes are to the left while gaseous nodes are to the right. To conserve space three of the gaseous species, as noted, are displayed on the left and should be associated with the gaseous nodes. Following is the key to the abbreviations:

F(C) - on left, solid fuel (I = 10); on right, gaseous pyrolyzed fuel (I = 1).

O(C) - on left, solid oxidizer (I = 11); on right, gaseous pyrolyzed oxidizer (I = 2).

P(C) - on left, product of solid reaction (I = 12); on right, gaseous pyrolyzed product of solid reaction (I = 3).

P(S, F+O(C)) - gaseous product of surface reaction between solid fuel and pyrolyzed oxidizer (I = 5).

P(S, F+O(G)) - gaseous product of surface reaction between solid fuel and initial gaseous oxidizer (I = 6).

INERT - gaseous inert diluent (I = 9).

O(G) = initial gaseous oxidizer (I = 4).

P(G, F+O(C)) - gaseous product of gas phase reaction between pyrolyzed fuel and pyrolyzed oxidizer (I = 7).

P(G, F+O(G)) - gaseous product of gas phase reaction between pyrolyzed fuel and initial gaseous oxidizer (I = 8).

Appendix A

GOVERNING EQUATIONS*

Field Equations (species and enthalpy)

Gas $(i = 1 - 9,13;\ \phi > 0)$

$$\frac{\partial Z_i}{\partial t} = A_i B_i (1-\phi)^2 \frac{\partial^2 Z_i}{\partial \phi^2} - A_i (1-\phi)\left(m_s + B_i\right) \frac{\partial Z_i}{\partial \phi} + V_i \qquad (A\text{-}1)$$

Solid $(i = 10 - 12, 14;\ B_i = 0,\ i = 10 - 12;\ \phi < 0)$

$$\frac{\partial Z_i}{\partial t} = A_i B_i (1+\phi)^2 \frac{\partial^2 Z_i}{\partial \phi^2} - A_i (1+\phi)\left(m_s - B_i\right) \frac{\partial Z_i}{\partial \phi} + V_i \qquad (A\text{-}2)$$

Interface

Species $(i = 1 - 9;\ m_{i+9} = 0,\ i > 3)$

$$m_{i+9} = m_s Z_i - B_i \frac{\partial Z_i}{\partial \phi} - S_i \qquad (A\text{-}3)$$

Enthalpy

$$B_{14} \frac{\partial Z_{14}}{\partial \phi} = B_{13} \frac{\partial Z_{13}}{\partial \phi} + S_{1314} \qquad (A\text{-}4)$$

Remote Boundary Conditions

Gas $(i = 1 - 9,\ 13)$

$$\frac{\partial Z_i}{\partial \phi}(1,t) = 0 \qquad (A\text{-}5)$$

Solid $(i = 10 - 12,\ 14)$

$$\frac{\partial Z_i}{\partial \phi}(-1,t) = 0 \qquad (A\text{-}6)$$

Initial Conditions $(i = 1 - 14)$

$$Z_i = Z_{io} \qquad (A\text{-}7)$$

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* See Ref. 1 for Nomenclature.

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Appendix B

REPRESENTATION OF GOVERNING EQUATIONS IN FINITE DIFFERENCE FORM

The finite difference formulation of the equations of Appendix A is based on the two step predictor-corrector algorithm described in Section 3. A finite difference net is established using equal spacing in the ϕ-space. The number of strips in the solid and gas phases is N_c and N_g, respectively, with nodal numbers running from one (solid remote boundary) to N_c+1 at the interface and continuing to N_c+N_g+1 at the gas phase remote boundary. The surface node is repeated to allow for surface discontinuities in species concentration. The spacing of the nodes is $\Delta\phi_1=1/N_c$ and $\Delta\phi_2=1/N_g$.

The predictor and corrector equations follow from Eq. (7-8) and take the following forms:

$$\frac{u_j^1 - u_j^o}{\Delta t/2} = f_{1i}(\phi_j)\left[u_{j+1}^1 - 2u_j^1 + u_{j-1}^1\right] + f_{2i}(\phi_j)\left[u_{j+1}^1 - u_{j-1}^1\right]g_i(u_s^o) + h_i(u_j^o) \qquad (B\text{-}1)$$

$$\frac{u_j^2 - u_j^o}{\Delta t} = f_{1i}(\phi_j)\left[u_{j+1}^2 - 2u_j^2 + u_{j-1}^2 + u_{j+1}^o - 2u_j^o + u_{j-1}^o\right]/2 + f_{2i}(\phi_j)\left[u_{j+1}^2 - u_{j-1}^2 + u_{j+1}^o - u_{j-1}^o\right]g_i(u_s^1)/2 + h_i(u_j^1) \qquad (B\text{-}2)$$

When unknowns are collected on the left and known quantities on the right, the following set of equations is obtained:

$$a_{ij}^k u_{j-1}^{k+1} + b_{ij}^k u_j^{k+1} + c_{ij}^k u_{j+1}^{k+1} = d_{ij}^k \qquad (B\text{-}3)$$

Where

$$a_{ij}^k = \left[-f_{1i}(\phi_j) + f_{2i}(\phi_j)g_i(u_s^k)\right]\Delta t/2 \qquad (B\text{-}4)$$

$$b_{ij}^k = 1 + f_{1i}(\phi_j)\Delta t \qquad (B\text{-}5)$$

$$c_{ij}^k = \left[-f_{1i}(\phi_j) - f_{2i}(\phi_j)g_i(u_s^k)\right]\Delta t/2 \qquad (B\text{-}6)$$

$$d_{ij}^k = h_i(u_j^k)\Delta t/2 \qquad (B\text{-}7)$$

for the predictor $(k = 0)$.

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The equations for a, b and c are unchanged for the corrector ($k=1$); the expression for d becomes:

$$d_{ij}^{k} = h_i\left(u_j^k\right)\Delta t + \left[f_{1i}\left(\phi_j\right) - f_{2i}\left(\phi_j\right) q_i\left(u_s^k\right)\right] u_{j-1}^{k-1}\,\Delta t/2 + \left[1 - f_{1i}\left(\phi_j\right)\Delta t\right] u_j^{k-1} + \left[f_{1i}\left(\phi_j\right) + f_{2i}\left(\phi_j\right) q_i\left(u_s^k\right)\right] u_{k+1}^{k-1}\,\Delta t/2 \qquad (B\text{-}8)$$

The finite difference forms of the interface equations are:

Gas species:

$$m_{i+9}^{k} = m_s^k u_{i,s}^{k+1} - B_i\left(u_{i,s+1}^{k+1} - u_{i,s-1}^{k+1}\right)/2\Delta\phi - S_i^k \qquad (B\text{-}9)$$

Elimination of u_{s-1} between Eq. (B-9) and (B-3) evaluated at $j=s$ (surface) provides the appropriate form for the tridiagonal matrix.

Solid species: Use the backward difference formula for $\partial u/\partial\phi$ in Eq. (A-2)

$$\frac{\partial u_s^k}{\partial\phi} = \left(u_{s-2}^k - 4u_{s-1}^k + 3u_s^k\right)/2\Delta\phi \qquad (B\text{-}10)$$

and eliminate u_{s-2} by use of Eq. (B-3) evaluated at $j = s-1$.

Enthalpy:

$$B_{14}\left(u_{14,s+1}^{k+1} - u_{14,s-1}^{k+1}\right)/2\Delta\phi_c = B_{13}\left(u_{13,s+1}^{k+1} - u_{13,s-1}^{k+1}\right)/2\Delta\phi_g + S_{1314}^k \qquad (B\text{-}11)$$

The quantities $u_{14,s+1}$ and $u_{13,s-1}$ represent fictitious nodes. They are eliminated by means of the solid enthalpy field equation for u_{13} and u_{14} centered at the surface. The resulting equation contains $u_{13,s}$ and $u_{14,s}$ related by

$$u_{13,s} = C_g u_{14,s}/C_c + C_g\left(T_{co} - T_{go}\right) \qquad (B\text{-}12)$$

which arises from continuity of temperature at the surface.

The result of the above operations is a set of tridiagonal equations to be solved for each of the twelve species and enthalpy for each half of the computing algorithm. There are N_c+1, N_g+1 and N_c+N_g+1 equations in the tridiagonal sets for solid species, gaseous species and enthalpy, respectively.

Appendix C

SAMPLE PRINTOUT OF COMPUTER CALCULATIONS

The following two pages show an example of the output produced by the computer program. The entire run is not reproduced.

The first page shows a matrix listing of the 80 NAMELIST variables and their associated numerical values. The particular values shown for FREQ 1, E1, Q1, COND (1), SPHT (1), RHO1, TLIM (1), YFZ1, and QDOT were chosen to duplicate a previous computation for solid phase ignition.[11] The interpretation of the final line on the first page is given in Section 4.2 (Program Input) paragraph (c).

The second page shows a sample output for the first five time steps. A complete explanation is given in Section 4.3 (Program Output). Since only solid phase calculations were made in this example, the results pertaining to the gas phase appear as zeros.

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[11] Bradley, H. H., Jr. "Theory of Ignition of a Reactive Solid by Constant Energy Flux," COMBUS SCI AND TECH, Vol. 2 (1970), pp. 11-20.

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CHECK RUN. SIMULATION OF SOLID PHASE REACTIONS. A=1.5+16, B=4.505, EPRIME=50.
15 JULY 74. DLLIM=.01, DULIM=.05
  FREQ1          FREQ5          FREQ6          FREQ7          FREQ8          FREQ10
 FREQ11         FREQ12          F1             E5             E6             F7
   F8             E10            F11            E12            Q1             Q5
   Q6             Q7             Q8             Q10            Q11            Q12
   VO7           VF7             VO8            VF8            SO5            SO6
  STOV2          STOV4          STOV11         STOS2          STOS4           MU1
   MU2            MU4            MU5            MU6            MU7            MU8
     MU9          MU10           MU11           MU12          COND(1)        COND(2)
 SPHT(1)        SPHT(2)           RHO1           LF             BE            TLIM(1)
 TLIM(2)         PRESS          YFZ1           YOZ2           QDOT           TMELIM
  TSLIM           FCI            NREFIR          TCO          CUTOFF           SUB
   REG          ALP(1)         ALP(2)          N(1)           N(2)           DULIM
  DLLIM          SPRO5          SPRO6         SPRO10         SPRO11         SPRO12
  NHLIM          SURF
 3.32960+15     0.00000        0.00000        0.00000        0.00000        0.00000
 0.00000        0.00000         99.350        0.00000        0.00000        0.00000
 0.00000        0.00000        0.00000        0.00000         4.5050        0.00000
 0.00000        0.00000        0.00000        0.00000        0.00000        0.00000
          1              1              1              1              1              1
  1.0000         1.0000         1.0000         1.0000         1.0000         1.0000
  1.0000         1.0000         1.0000         1.0000         1.0000         1.0000
  1.0000         1.0000         1.0000         1.0000         1.0000         1.0000
  1.0000         1.0000         1.0000         1.0000         1.0000         1.0000
  1.0000         82.050         .50000         1.0000         1.0000         .14000
  3.2000         2.0000                 0     11.000                 F              F
          F      2.0000        0.00000               100            100    5.00000-02
 1.00000-02              0              0              0              0              0
         10              F

000000000011101   50 29 12  5  2  1  0  0  1  2  5 12 29 50  1100000      .100
```